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DEVELOPMENT OF AN X-RAY TRANSPORT MODEL BASED ON PEIERLS' INTEG--ETC(U)
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AN X-RAY TRANSPORT MODEL

BASED ON PEIERLS' INTEGRAL EQUATION.

THESIS

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DEVELOPMENT OF
AN X-RAY TRANSPORT MODEL
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THESIS

Presented to the Faculty of the School of Engineering
of the Air Force Institute of Technology
Air University
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Requirements for the Degree of
Master of Science

by

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March 1980

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Preface

This report contains the results of my efforts to develop a model for time-dependent x-ray transport in air. I have tried to present a complete description of the derivation of the equations, the assumptions made, and the complexities involved in trying to devise a set of numerical difference equations to solve the model efficiently.

There are several people to whom I am indebted and owe thanks. First, I would like to thank my advisor, Major George H. Nickel, for without his help, guidance, and encouragement I would not have completed the study. I would also like to thank Doctor Charles J. Bridgman and Captain David D. Hardin to whom I frequently went for advice. Lastly, I thank my wife, Yuao-Ching, for her patience, love, and understanding throughout the period of this work.

Robert P. Dickey

(This thesis was typed by Sharon A. Gabriel)

Contents

List of Figures

Notation

W	Relative kinetic energy of the electrons
e	Electron charge
b	Impact parameter
b_0	Impact parameter for single interaction, 90 degree deflection
σ_c	Cross section for short-range encounter
λ_d	Debye shielding distance
k	Boltzmann constant
T	Kinetic temperature
n_e	Electron number density
n_i	Ion number density
σ_d	Cross section for long-range encounter
W^*	Actual energy of scattered particle
Λ	Debye shielding distance divided by the impact parameter for a single interaction, 90 degree deflection
v_e	average electron velocity

Notation (Cont'd)

v_i	Average ion velocity
λ	Absorption mean free path of air at burnout temperature
t_{ee}	Mean collision time between electron-electron scatters
t_{ei}	Mean collision time between electron-ion scatters
t_p	Equilibrium time for thermal photons
Y	Source strength
α	Parameter for source growth
β	Parameter for source decay
t_0	Parameter for the time when the maximum x-ray energy is emitted from the source
Z	Normalization constant for source time dependence
f(t)	Source time dependence function
$E_s(R,t)$	Streaming radiation density at position R, time t
$F_s(R,t)$	Streaming radiation flux at position R, time t
$E_t(R,t)$	Thermal radiation density at position R, time t

Notation (Cont'd)

$F_t(R,t)$	Thermal radiation flux at position R, time t
$E_m(R,t)$	Material energy density of air at position R, time t
$T(R,t)$	Kinetic air temperature at position R, time t
c	Speed of light
κ_s	Mean opacity of air at the burnout temperature for streaming x-rays
κ_t	Mean opacity of air at the burnout temperature for thermal x-rays
T_B	Burnout temperature of air
ρ	Density of air
σ	Stefan-Boltzmann constant
S	Path length from R' to R equal to $\|R'-R\|$
a	Radiation constant
T_{eff}	Effective thermal radiation temperature
C_v	Air heat capacity
μ_ℓ	Direction cosines for Gaussian quadrature
ω_ℓ	Weights associated with direction cosines μ_ℓ

Abstract

An x-ray transport model is developed which gives the streaming radiation flux, thermal radiation flux, and material energy of air, as a function of both position and time, following the release of a large amount of x-ray energy in the atmosphere. The model is intended as a compromise between the simple diffusion theory models and the accurate transport theory models. It applies to the radiative growth which takes place at early times before hydrodynamic motion begins. The model assumes that air is heated by photoelectric absorptions to a burnout temperature, the kinetic temperature at which the air molecules are completely ionized. The opacity of air is assumed very large at temperatures below the burnout temperature and very small at temperatures above the burnout temperature. Peierls' integral equation is used to calculate the flux of thermal radiation which builds up in the burned-out sphere of air. The integral equation considers both the nonlocal and retarded time-dependent characteristics of the thermal radiation field. An efficient numerical solution to the model is greatly complicated due to the inverse cubic temperature dependence of the opacity and the retarded time dependence of the thermal radiation field. A numerical algorithm is presented for solving the model.

DEVELOPMENT OF

AN X-RAY TRANSPORT MODEL

BASED ON PEIERLS' INTEGRAL EQUATION

I. Introduction

The point source release of a large amount of x-ray energy in the atmosphere initiates an extremely complex series of physical processes in which the x-ray energy liberated by the source heats the air, and the air then radiates to cool itself. The competition between the various modes of energy transport and the complexities of the radiation properties of air make a direct analytic attack infeasible (Ref 1:2). The usual approach is to use transport theory and obtain numerical solutions to the equation of transfer, also called the transport equation.

The transport equation is an integro-differential equation which is a mathematical statement of the gains and losses of photons. Even for one-dimensional systems with spherical symmetry, the transport equation expresses the specific intensity of radiation as a function of four independent variables: position, frequency, direction, and time. A typical x-ray transport problem might involve up to 50 or more radial zones and perhaps 10 frequency groups and 10 directions. In the numerical solution to this

problem, each combination of position, frequency, and photon direction requires a separate mesh point. The calculation is entirely nonlocal in that photons emitted at any one mesh point at a specific time can contribute to the number of photons at any other mesh point at a later time. Clearly, to solve this problem numerically would require extensive computer time and storage capability.

An alternative approach to solving the x-ray transport problem would be to use diffusion theory. Diffusion theory assumes that the radiative flux is proportional to the gradient of the thermal radiation energy density. Although this assumption is very crude, it is a widely used approximation in radiation transport calculations because of its simplicity (Ref 2:51). Unlike transport theory, diffusion theory is strictly local in the sense that the number of photons at any one mesh point can only be influenced by the closest neighboring mesh points. If the photon mean free path is small compared to the dimensions of the system, then diffusion theory may be applicable. However, for most optically thin spherical systems this is not the case and diffusion theory does not apply.

A different approach to the x-ray transport problem would be to solve an integral form of the transport equation often referred to as "Peierls' Equation" (Ref 2:31). Peierls' equation solves for the all-angle thermal radiation flux in a system which scatters photons isotropically, and therefore

it contains two less independent variables which describe direction in the full equation of transfer. The actual thermal radiation flux may or may not be isotropic. A form of the integral equation can be derived for time-dependent radiative transfer which accounts for the nonlocal effect of the radiation field. An efficient numerical solution of Peierls' equation should improve upon the accuracy and simplicity of diffusion theory models without using as much computer time and storage capability as the full transport theory models.

PURPOSE

The purpose of this thesis was to develop a model that would describe the radiative transport process which takes place following the release of a large amount of x-ray energy in the atmosphere. The intention was to develop a model that would improve upon the accuracy of diffusion theory models while reducing the computer time needed by full transport theory models. A model based on Peierls' integral equation will be developed and analyzed to see if it satisfies thc above criteria.

SCOPE

This model describes one-dimensional, time-dependent x-ray transport, in spherical geometry, for the point source release of a large amount of x-ray energy in the atmosphere.

The model applies at very early times before shock formation and hydrodynamic expansion takes place. Rather than treat the photon frequency as a continuous variable, all photons will be grouped together and average properties assigned.

ASSUMPTIONS

The following assumptions have been made to clarify and simplify the x-ray transport model:

1. The source emits x-rays isotropically.
2. The scattering of x-rays is isotropic.
3. The density of air is uniform at its ambient value because of the absence of hydrodynamic motion during early time periods.
4. The opacity of air has an inverse cubic temperature dependence.

OVERVIEW

This report contains five sections and one appendix. Section II gives a theoretical background description of the physical processes taking place during x-ray transport. Based on the underlying physics, the equations needed to solve the model are developed in Section III. In Section IV, the resulting model is discussed and compared to an existing diffusion theory model. Finally, the conclusions and recommendations are presented in Section V. Appendix A describes a numerical algorithm which could be used to solve the model.

II. Background

This section presents a background description of what physically takes place when a large amount of x-ray energy is released in the air. A discussion of the underlying physics of x-ray transport in air will help to account for assumptions and equations presented later in the development of the model. Much of the discussion comes from the work of Glasstone (Ref 3), and Pomraning (Ref 4), who dealt with x-ray transport as it pertains to nuclear weapon effects. The ionization of the air will be discussed first, followed by an estimation of the time required to form a Maxwell-Boltzmann distribution of electrons and ions.

IONIZATION OF AIR

Initially, an intense point source emits x-rays with several KEVs of energy into the atmosphere. Close to the source, the x-rays which arrive first will strip off electrons from the air molecules due to photoelectric absorptions. As more electrons are stripped from the air molecules, the air begins to heat up until it reaches what is called the burnout temperature. The burnout temperature is the kinetic temperature ascribed to the system of completely ionized air molecules whose velocity distribution

is Maxwellian. Photoelectric absorption is no longer possible in the completely ionized air and thus an upper limit exists on the amount of x-ray energy which can be deposited in a given volume of air. The air opacity is assumed to be very large for temperatures below the burnout temperature and very small for temperatures above the burnout temperature (Ref 4:220). As the source continues to emit x-rays, the spherical region of completely ionized air around the source expands and grows.

Inside the burned-out sphere, the heated air begins to radiate and cool down. Electrons that were stripped from air molecules emit bremsstrahlung radiation. Photons and moving electrons interact by compton and inverse compton scattering. As the kinetic air temperature cools below the burnout temperature, the opacity of air increases, and more source x-rays are then absorbed maintaining the air at the burnout temperature. The net result of these various interactions is the buildup of a thermal radiation field in the burned-out sphere. For systems whose dimensions are on the order of the mean free path for absorption of photons, the actual thermal radiation from the medium will be of the order of the blackbody value (Ref 5:28). Normally, "temperature" implies thermodynamic equilibrium, which means both kinetic and blackbody radiation equilibrium (Ref 5:28). The term "kinetic temperature" has been used here because the effective thermal radiation temperature

will initially be much lower than the kinetic temperature of the air particles, resulting in a two-temperature problem.

Growth of the burned-out sphere due to source x-rays will continue until the source strength is insufficient to both continue ionizing new layers of air and maintain the cooling air at the burnout temperature. This is the end of the burnout phase and further growth takes place through a diffusion process (Ref 4:220). At this time the ionized air is at a fairly uniform temperature, although temperature gradients do exist, particularly near the advancing radiation front (Ref 3:65). The thermal radiation field continues building up in the burned-out volume of air. The absorption of the thermal radiation in the surrounding cold air causes the diffusive growth. The source is no longer capable of keeping the air hot, and as the air temperature decreases, the photon mean free path decreases and growth of the ionized sphere becomes less rapid. Eventually, the effective thermal radiation temperature and the material kinetic temperature of the air will approach each other as the radiation and material tend toward equilibrium (Ref 4:225).

FORMATION OF A MAXWELL-BOLTZMANN DISTRIBUTION

An estimate of the time required for the electrons and ions to reach a Maxwellian distribution is needed to

justify using a Maxwell-Boltzmann equilibrium expression for the material energy density of the air. Glasstone and Lovberg define a collision as a coulomb force interaction which results in a deflection of more than 90 degrees (Ref 5:83). This collision can be a single interaction between a pair of charged particles (a short-range encounter) or a combined net effect due to multiple interactions between a single particle and many other particles (a long-range encounter) (Ref 5:83).

To determine the cross section for a short-range encounter, Glasstone defines the impact parameter for a 90 degree scatter, b_0, as the distance of closest approach between two particles in the absence of any electrostatic forces (Figure 1). From Coulomb's Law, it is found that the particles are a distance $2b_0$ apart at the point of closest approach for a 90 degree scatter, and that at this distance the mutual coulomb energy is equal to the center-of-mass (or relative) kinetic energy of the interacting particles (Ref 5:88). For the case of two charged particles carrying the unit electron charge e, (Ref 5:88):

$$W = \frac{e^2}{2b_0} \qquad \text{or} \qquad b_0 = \frac{e^2}{2W} \text{ cm} \tag{2.1}$$

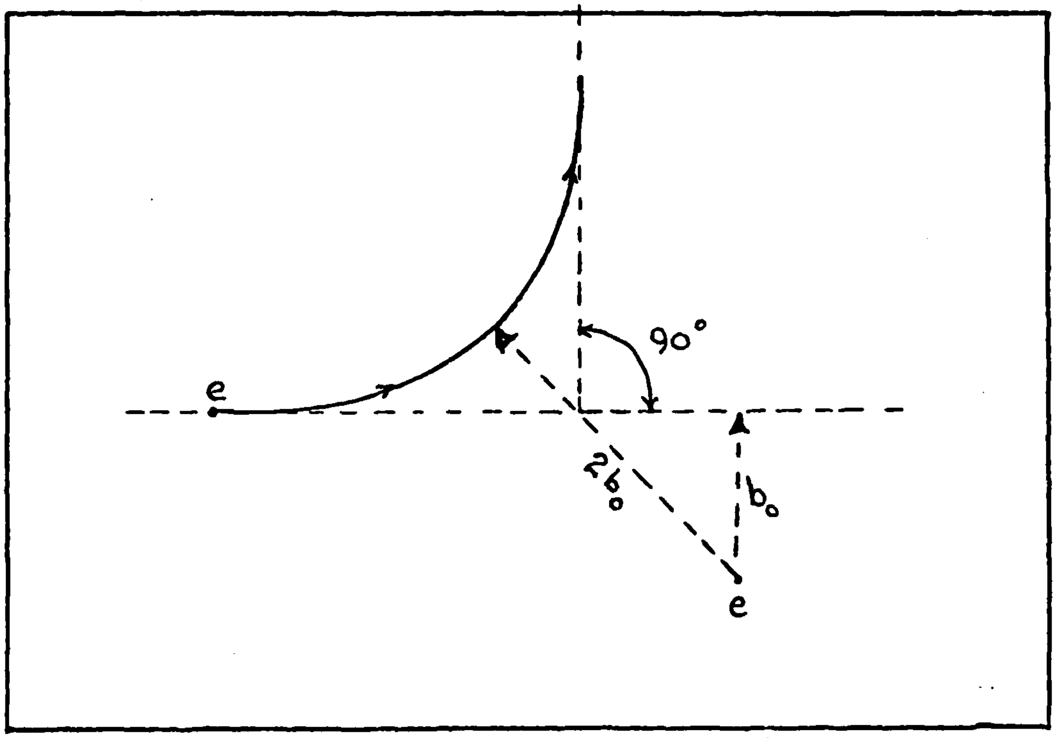

Figure 1. Short-Range Coulomb Interaction for 90 Degree Deflection (Ref 5:88)

where

W = relative kinetic energy of the particles in ergs

e = electron charge in statcoulombs.

The cross section for the short-range encounter, σ_c , can be estimated as the area of a disc of radius b_0 (Ref 5:88),

$$\sigma_c \simeq \pi b_o{}^2 = \frac{\pi e^4}{4W^2} \tag{2.2}$$

In analyzing the scattering collision, on a microscopic scale, due to long-range encounters, every charged particle may be regarded as being surrounded by an atmosphere having a net charge of the opposite sign (Ref 5:84). By postulating that the charged particles have a Boltzmann distribution, and assuming the gradient of the electric potential can be expressed by Poisson's equation based on Coulomb's Law, the effective radius of the oppositely charged atmosphere surrounding a positive ion can be shown to be (Ref 5:85):

$$\lambda_d = \left[\frac{kT}{4\pi n_e e^2}\right]^{\frac{1}{2}} = 2.35 \times 10^4 \left[\frac{T\,(Kev)}{n_e\,(\#/cm^3)}\right]^{.\frac{1}{2}} \text{cm} \tag{2.3}$$

where

λ_d = Debye shielding (or screening) distance

k = Boltzmann constant

T = kinetic temperature of both electrons and positive ions assuming a Maxwell-Boltzmann distribution

n_e = electron number density.

The cross section for a long-range encounter is estimated by determining the momentum change that results from the coulomb force at the distance of the impact parameter b , operating over a path length $2b$, for a time $2b/v$, where v is the velocity of the scattered particle (Ref 5:91). The particle is assumed to have been scattered through a large angle, about 90 degrees, when the average of the square of the total momentum change, $\overline{(\Delta P)^2}$, has increased to the point that it is roughly equal to the square of the initial momentum of the scattered particle, P^2 (Ref 5:92). The distance traveled by the particle is equivalent to a mean free path for the scattering process, and it is possible to define a cross section for the long-range encounter, σ_d , as (Ref 5:93)

$$\sigma_d \simeq \frac{2\pi e^4}{W^{*2}} \ln\Lambda \tag{2.4}$$

where

$$\Lambda \simeq \frac{\lambda_d \text{ (Debye shielding distance)}}{b_o \text{ (Impact parameter for a 90° scatter, for a short-range encounter)}}$$

W^* = actual energy of the scattered particle taken to be 3/2 kT if energy distribution is Maxwellian.

Substituting Eq (2.1) and (2.3) for b_0 and λ_d, respectively, gives

$$\sigma_d \simeq \frac{2\pi e^4}{W^{*2}} \ln \left[\frac{2.35 \times 10^4 \left(\frac{T\,(\text{kev})}{n_e\,(\#/\text{cm}^3)} \right)^{\frac{1}{2}}}{\frac{e^2}{2W}} \right] \tag{2.5}$$

Assuming the ionized atmosphere consists of electrons and nitrogen ions, with

e = 4.8×10^{-10} esu

T = .4 kev (the burnout temperature of air)

n_e $\simeq$ 3.76×10^{20} electrons/cm^3

W $\simeq$ 1.9×10^{-9} ergs

W^* $\simeq$ 9.6×10^{-10} ergs

gives

$$\sigma_d \simeq 3.4 \times 10^{-18}\ \text{cm}^2 \ .$$

The mean collision time between electron-electron scatters, t_{ee}, can now be estimated as (Ref 5:95)

$$t_{ee} = \frac{1}{n_e \sigma_d v_e} = 5.4 \times 10^{-13} \text{ sec} \tag{2.6}$$

where $v_e \approx 1.45 \times 10^9$ cm/sec (average electron velocity). Similarly, the mean collision time between ion-ion scatters, t_{ii}, can be estimated as (Ref 5:97)

$$t_{ii} = \frac{1}{n_i \sigma_d v_i} = 6.0 \times 10^{-10} \text{ sec} \tag{2.7}$$

where

$n_i \simeq 5.37 \times 10^{19}$ ions/cm^3

$v_i \simeq 9.1 \times 10^6$ cm/sec (average ion velocity).

Finally, the mean collision time between electron-ion scatters, t_{ei}, can be estimated as (Ref 5:97)

$$t_{ei} = \frac{1}{n_i \sigma_d v_e} = 3.8 \times 10^{-12} \text{ sec} \tag{2.8}$$

The time required for several collisions between electrons and ions is so short compared to the time dependence for source emission of x-rays, which is typically on the order of shakes (10^{-8} sec), that essentially a Maxwell-Boltzmann distribution forms instantaneously.

An interesting comparison can be made by estimating the equilibration time, t_p, for thermal photons to be

$$t_p = \frac{\lambda}{c} \tag{2.9}$$

where

λ = absorption mean free path of air at burnout temperature

c = speed of light

For $\lambda \simeq 50$ meters (Ref 4:225)

$$t_p = 1.67 \times 10^{-7} \text{ sec}$$

While the air particles reach a Maxwell-Boltzmann distribution on the order of 10^{-10} seconds, the thermal photons reach equilibrium on the order of 10^{-7} seconds, giving a two-temperature problem with the thermal radiation field initially not in equilibrium with the particles.

III. Development of X-Ray Transport Model

This section derives in spherical geometry the equations needed to describe the transport of a large amount of x-ray energy released in the air. Three questions are developed, one each for the streaming radiation flux, thermal radiation flux, and material energy of air. The three variables depend not only on time, but also on radial position. The equation for the streaming radiation flux describes a point source that has been exponentially attenuated and spherically diverged. A form of Peierls' integral equation will be derived to calculate the thermal radiation flux, and the material energy of air will be determined by writing a rate equation which accounts for the gains and losses of material energy.

The source time dependence and its properties will be described first, followed by the derivations of the streaming radiation flux, thermal radiation flux, and material energy of air, respectively. The end of this section will show how energy is conserved in the model.

SOURCE TIME DEPENDENCE

Assume a point source of radiation of source strength Y, and a time dependence, $f(t)$, given by Pomraning as (Ref 6:3)

$$f(t) = \frac{1}{Z} \frac{(\alpha+\beta)e^{\alpha(t - t_o)}}{\beta+\alpha\ e^{(\alpha+\beta)(t - t_o)}} \tag{3.1}$$

where

α = parameter for source growth

β = parameter for source decay

t_o = parameter for the time when the maximum x-ray energy is emitted from the source

Z = normalization constant such that the $\int_0^\infty f(t)\,dt = 1$.

It is assumed that the source emits a Planck blackbody spectrum of x-rays into an infinite sea of uniform-density air. The time dependence for source emission of x-rays has the following properties (Ref 6:3):

(a) Rises like $e^{\alpha t}$ for small t ;

(b) Falls like $e^{-\beta t}$ for large t ;

(c) Has a single maximum at $t = t_o$;

(d) $f(t_o) = \frac{1}{Z}$.

STREAMING RADIATION FLUX

The streaming radiation at position R , time t , includes only those virgin x-rays which were emitted by the source at an earlier time and arrived untouched at position R at time t . An energy balance is performed for the

streaming radiation density in ∂r about position R , and in ∂t about time t (Ref 6:6).

$$\underbrace{4\pi R^2 E_s(R,t)\; c\; \partial t}_{\text{Streaming Radiation In}}\Big|_{r} - \underbrace{4\pi R^2 E_s(R,t)\; c\; \partial t}_{\text{Streaming Radiation Out}}\Big|_{r+\partial r} = \underbrace{4\pi R^2 \partial r\; d[E_s(R,t)]}_{\text{Streaming Radiation Absorbed}} \qquad (3.2)$$

Here c is the speed of light and $E_s(R,t)$ is the streaming radiation density at position R , time t . Eq (3.2) gives the result that (Ref 6:7)

$$\frac{\partial}{\partial r}\left[4\pi R^2 E_s(R,t)c\right] = 4\pi R^2 \frac{\partial}{\partial t}\left[E_s(R,t)\right] \qquad (3.3)$$

The streaming radiation emitted by the source at time t can only decrease due to absorption by the air as it streams away from the source. Recall the opacity of air was assumed very large at temperatures below the burnout temperature and very small at temperatures above the burnout temperature. It is now assumed that the specific temperature dependence of the opacity is given by (Ref 6:15)

$$\kappa(R,t) = \kappa\left[\frac{T_B}{T(R,t)}\right]^3 \qquad (3.4)$$

where

$\kappa(R,t)$ = the opacity of air at position R, time t, which depends on the air temperature at position R, time t.

κ = the opacity of air at the burnout temperature (a constant).

T_B = burnout temperature of air

$T(R,t)$ = the kinetic air temperature at position R, time t

The time rate of change of $E_s(R,t)$ can therefore be expressed as

$$\frac{\partial}{\partial t}\left[E_s(R,t)\right] = -\rho\kappa_s\left[\frac{T_B}{T(R,t)}\right]^3 E_s(R,t)c \tag{3.5}$$

where ρ is the density of air, assumed constant, and κ_s is the mean opacity of air at the burnout temperature for streaming x-rays being emitted by a Planckian source. The right side of Eq (3.5) is simply the rate at which streaming radiation density is absorbed by the air.

Equation (3.3) can now be written with the right side of Eq (3.5) substituted in for the time rate of change of the streaming radiation energy density, giving

$$\frac{\partial}{\partial r}\left[4\pi R^2 E_s(R,t)c\right] = -4\pi R^2\rho\kappa_s\left[\frac{T_B}{T(R,t)}\right]^3 E_s(R,t)c \tag{3.6}$$

and solved with an integrating factor to give

$$4\pi R^2 E_s(R,t)c \quad = \quad D\, e^{-\int_0^R \rho\kappa_s \left[\frac{T_B}{T(r,t\,-\,\frac{R-r}{c})}\right]^3 dr} \tag{3.7}$$

The constant of integration, D, can be determined from the boundary condition for an arbitrarily small sphere surrounding the source (Ref 6:7)

$$4\pi R^2 E_s(R,t)c \xrightarrow[R\to 0]{} Yf(t) \tag{3.8}$$

giving the result that

$$E_s(R,t)c \quad = \quad \frac{Yf(t-R/c)}{4\pi R^2}\, e^{-\int_0^R \rho\kappa_s \left[\frac{T_B}{T(r,t-\frac{R-r}{c})}\right]^3 dr} \tag{3.9}$$

Notice that Eqs (3.7) and (3.9) include the necessary time retardation which accounts for the finite speed of light and the dependence of the air temperature on the path-length variable r, in the exponential attenuation term. A final reduction can be made to Eq (3.9) by recognizing that

$$E_s(R,t)c \quad = \quad R_s(R,t) \tag{3.10}$$

where $F_s(R,t)$ is the streaming radiation flux at position

R , time t . The equation for the streaming radiation flux can now be written in final form as

$$F_s(R,t) = \frac{Yf(t-R/c)}{4\pi R^2} e^{-\int_0^R \rho\kappa_s \left[\frac{T_B}{T(r,t-\frac{R-r}{c})}\right]^3 dr} . \qquad (3.11)$$

The streaming radiation flux at position R , at time t , is simply the source strength emitted at an earlier time, exponentially attenuated and spherically diverged to arrive at position R , at time t .

THERMAL RADIATION FLUX

The thermal radiation flux which builds up in the optically thin, heated air will now be considered. This consideration must include both the nonlocal and retarded time dependent characteristics of the thermal radiation field. The development of the equation for the thermal radiation flux follows an analogous development by Weinberg and Wigner for an integral equation for the transport of monoenergetic neutrons (Ref 7:182).

First, a differential volume element in the shape of a flat disc is positioned at R , with its axis in the direction from R' to R (Figure 2). The thermal radiation being emitted at position R' , at time t , can be expressed as

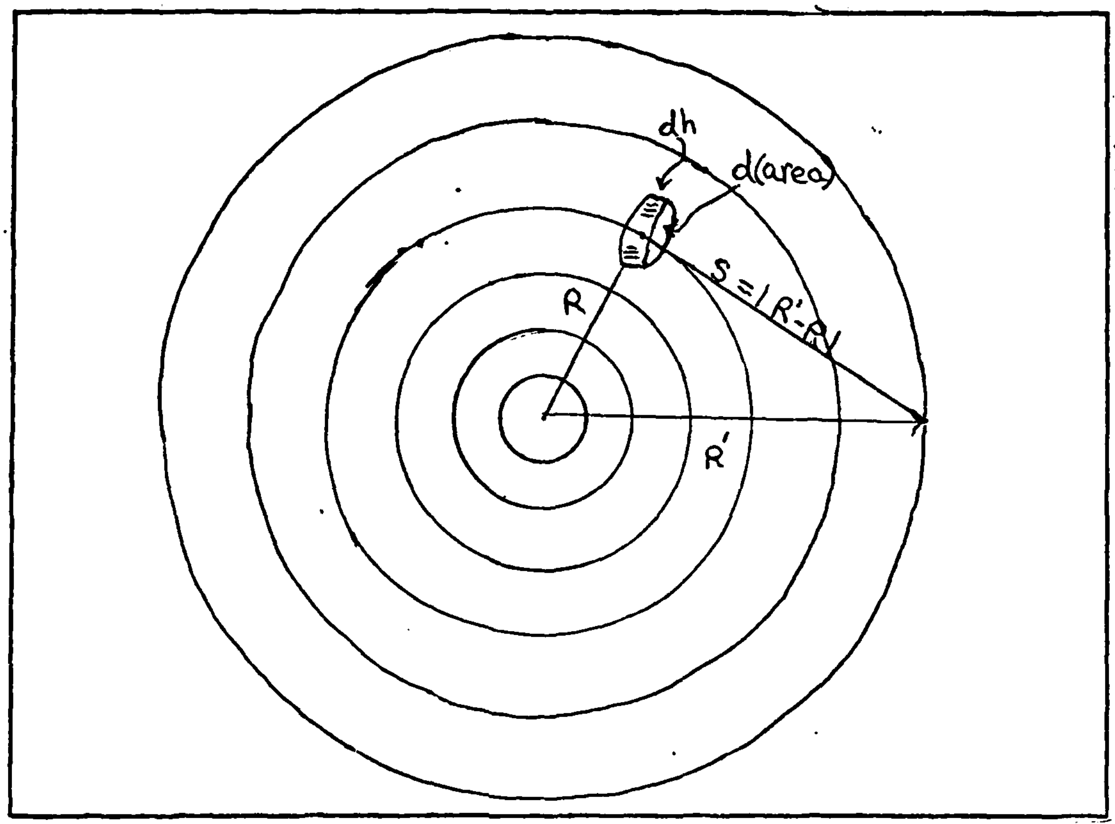

Figure 2. Geometry Associated with Thermal Radiation Flux

$$\rho \kappa_t \left[\frac{T_B}{T(R',t)} \right]^3 caT(R',t)^4 \qquad (3.12)$$

where "a" is the radiation constant and κ_t is the mean opacity of air at the burnout temperature for thermal x-rays. In order to arrive at position R , at time t , photons had to be emitted in the solid angle $d(area)/4\pi S^2$, at an earlier time, $t - S/c$, where S is the path length from R' to R , and d(area) is the differential area of the base of the disc (Figure 2). The probability

that photons arrive at the disc without undergoing further attenuation is

$$e^{-\int_0^S \rho\kappa_t \left[\frac{T_B}{T(R',t-S'/c)}\right]^3 dS'} \tag{3.13}$$

Since the height of the disc is equal to dh, the sum of the path lengths of the photons in the disc at time t, due to photons emitted earlier at position R' is

$$\rho\kappa_t \left[\frac{T_B}{T(R',t-S/c)}\right]^3 caT(R',t-S/c)^4 \frac{d(\text{area})dh}{4\pi S^2} e^{-\int_0^S \rho\kappa_t \left[\frac{T_B}{T(R',t-S'/c)}\right]^3 dS'} \tag{3.14}$$

Equation (3.14), divided by the volume of the disc, $d(\text{area})dh$, is the contribution to the thermal radiation flux at position R, at time t, due to radiation emitted earlier from position R'. The total, all-angle thermal radiation flux, at position R, at time t, $F_t(R,t)$, will be the integral of Eq (3.14) over the entire volume, namely

$$F_t(R,t) = \int dVOL \frac{\rho\kappa_t \left[\frac{T_B}{T(R',t-S/c)}\right]^3 caT(R',t-S/c)^4}{4\pi S^2}$$

$$\times \quad e^{-\int_0^S \rho\kappa_t \left[\frac{T_B}{T(R',t-S'/c)}\right]^3 dS'} \tag{3.15}$$

Equation (3.15), integral in character, describes time dependent radiative transfer in a system which isotropically scatters photons. The actual flux itself will not be isotropic, especially near the boundaries. The equation is of a form commonly referred to as Peierls' equation (Ref 2:31). The fact that the opacity depends on one of the dependent variables, the kinetic air temperature, greatly complicates the solution to Eq (3.15). It will be useful to define an effective temperature for the thermal radiation field, T_{eff}, from the relationship

$$\sigma T_{eff}(R,t)^4 = F_t(R,t) \tag{3.16}$$

where σ is the Stefan-Boltzmann constant.

MATERIAL ENERGY DENSITY

The material energy density of air is simply the kinetic energy of the ions and electrons. In a given molecular system, the exchange of energy between colliding ions and electrons causes the presence of a Maxwell-Boltzmann distribution of energies. Earlier, it was shown that a Maxwell-Boltzmann distribution of electrons and ions forms almost instantaneously following the release of a large amount of x-ray energy in the air. Therefore, based on the assumption that the molecular air is in equilibrium with a Maxwell-Boltzmann distribution of energies, the

material energy density of air at any position R , and time t , can be expressed by the relationship

$$E_m(R,t) = C_v T(R,t) \tag{3.17}$$

where $E_m(R,t)$ is the material energy density of air, and C_v is the heat capacity of air, assumed constant (Ref 4:223). The real unknown is the kinetic air temperature, since the material energy density is known if the temperature is known.

Three processes are taking place which affect the temperature of air. The temperature of air is increased when either streaming radiation or thermal radiation is absorbed, and is decreased when the air radiates to cool itself. An equation is written for the time rate of change of the material energy density due to these gains and losses.

$$\begin{aligned}\frac{\partial}{\partial t}[E_m(R,t)] = C_v\frac{\partial}{\partial t}[T(R,t)] &= \rho\kappa_s\left[\frac{T_B}{T(R,t)}\right]^3 F_s(R,t) \\ &+ \rho\kappa_t\left[\frac{T_B}{T(R,t)}\right]^3 F_t(R,t) \\ &- \rho\kappa_t\left[\frac{T_B}{T(R,t)}\right]^3 caT(R,t)^4\end{aligned} \tag{3.18}$$

An iterative process will be required to numerically solve for the unknown air temperature in Eq (3.18).

CONSERVATION OF ENERGY

This x-ray transport model was developed from the basic principle of energy conservation. At any time t , the total streaming radiation energy, thermal radiation energy, and material energy, contained in the volume of air, must equal the total energy emitted by the source up to time t . When streaming radiation or thermal radiation is attenuated by absorption, the material energy of air must increase. Likewise, when the air radiates to cool itself, thermal radiation energy must increase while material energy must decrease.

On inspecting the equations for the streaming radiation flux, thermal radiation flux, and material energy density of air, it is not obvious that energy is conserved. In order to show that energy is conserved, the equations for the streaming radiation and the thermal radiation are expressed as energy densities instead of fluxes. The three energy density equations are now

$$E_s(R,\cdot) = \overset{\textcircled{1}}{\frac{Yf(t-R/c)}{4\pi R^2 c}}\, e^{-\int_0^R \rho\kappa_s \left[\frac{T_B}{T\left(r,t-\frac{R-r}{c}\right)}\right]^3 dr} \tag{3.19}$$

$$E_t(R,t) = \frac{4}{c}\int dVOL\, \frac{\rho\kappa_t \left[\frac{T_B}{T(R',t-S/c)}\right]^3 \overset{\textcircled{2}}{caT(R',t-S/c)^4}}{4\pi S^2} \times e^{-\int_0^S \rho\kappa_t \left[\frac{T_B}{T(R',t-S'/c)}\right]^3 dS'} \tag{3.20}$$

$$E_m(R,t) = E_m(R,t-1) + \Delta t \left[\rho \kappa_s \left[\frac{T_B}{T(R,t)} \right]^3 F_s(R,t) \right.$$

$$+ \rho \kappa_t \left[\frac{T_B}{T(R,t)} \right]^3 F_t(R,t)$$

$$\left. - \rho \kappa_t \left[\frac{T_B}{T(R,t)} \right]^3 caT(R,t)^4 \right] \qquad (3.21)$$

where the time rate of change of the material energy density was replaced by a backward difference equation and $E_t(R,t)$, which is the thermal radiation density at position R and time, defined from the relationship

$$\frac{c}{4} E_t(R,t) = F_t(R,t) \qquad (3.22)$$

Conservation of energy is now determined by integrating the three equations over the entire volume and adding them up. Integrating and adding up the left-hand sides of Eqs (3.19), (3.20), and (3.21) gives the total streaming radiation energy, thermal radiation energy, and material energy in the volume at time t . On integrating and adding up the right-hand sides of Eqs (3.19), (3.20), and (3.21),

it is found that the exponential attenuation portion of Eq (3.19), integrated over the volume, is cancelled by the material energy gains due to streaming radiation absorption, terms 3 and 4 Eq (3.21). Similarly, the emission and exponential attenuation portions from the thermal radiation energy, term 2 Eq (3.20), are cancelled by terms 3 , 5 , and 6 , in Eq (3.21) when integrated over the entire volume. What remains after adding up all terms is only the source strength emitted up to time t in term 1 of Eq (3.19). Energy is conserved since the total streaming radiation energy, thermal radiation energy, and material energy is equal to the source strength emitted up to time t .

IV. Results and Discussion

In this section the x-ray transport model developed from Peierls' integral equation will be analyzed. Recall, the intention was to develop a model that would improve upon the accuracy of diffusion theory models while reducing the computer time required of full transport theory models. Based on that criterion, the model developed in this study will be compared to an existing diffusion theory model by Pomraning (Ref 6). A qualitative measure of the accuracy will be made by comparing the basic theory and assumptions on which each model is based. The model developed in this study will then be numerically analyzed to see if the model lends itself to an efficient numerical solution.

COMPARISON TO POMRANING'S DIFFUSION THEORY MODEL

Pomraning develops a relatively straightforward model for the release of a large amount of x-ray energy in the atmosphere by assuming two distinct phases for the growth of the ionized sphere of air (Ref 4:220). The initial phase, or burnout phase, consists of the complete ionization and burnout of the air, followed by a diffusive growth phase which begins when the source of x-rays can no longer maintain the air at the burnout temperature. The final conditions that exist at the end of the burnout phase become

the initial conditions for the start of the diffusive growth phase. In reality there are not two distinct phases, but a smooth blending from one phase to the next. The model developed in this study does not separate the two phases, but allows them to blend smoothly together.

In Pomraning's burnout phase, he assumes the sphere to be optically thin and therefore he ignores spatial gradients and writes rate equations for the volume as a whole (Ref 4:221). He advances a radiation front with an associated burnout radius. Inside, the burnout radius is completely ionized air at the burnout temperature, while outside the burnout radius is ambient air. The model developed in this study also assumes an optically thin sphere, but spatial gradients are not ignored. The thermal radiation flux, streaming radiation flux, and kinetic air temperature are all determined as a function of both position and time. According to Glasstone (Ref 3:65), temperature gradients do exist, particularly near the advancing radiation front. If temperature gradients exist, then thermal radiation gradients would also exist, and a numerical solution to this model would give a good indication of the magnitude of these gradients. Since the kinetic air temperature is determined as a function of position and time, it is no longer necessary to advance a radiation front with an associated burnout radius. The spatial dependence of the air temperature will indicate the volume of air that is completely ionized, as well as the regions that are only partially ionized.

After completion of the burnout phase, Pomraning uses diffusion theory to model further growth of the ionized sphere of air. To obtain diffusion theory, he assumes the radiative flux is proportional to the gradient of the thermal radiation energy density (Ref 4:223). Diffusion theory is most accurate when the dimensions of the system are large compared to the photon mean free path. For a spherical system of ionized air with a radius in the tens of meters, all points in the system are within a few mean free paths. Pomraning also assumes that the kinetic air temperature, the thermal radiation density, and the streaming radiation density are all space independent within the sphere of ionized air, and zero elsewhere (Ref 4:224). Instead of the diffusion equation, this model was developed around Peirels' integral equation. Peirels' equation gives spatial dependence while accounting for the time retardation and nonlocal characteristics of the radiation field. The accuracy of Peierls' equation is not dependent on the photon mean free path or the nearness of a calculation to a boundary.

NUMERICAL ANALYSIS

Before proceeding directly into the numerical analysis, some introductory comments will be made on the numerical approach to solving this model. The initial idea for using an integral equation of Peierls' form came from the

similarity of Peierls' integral equation to the integral from of the neutron transport equation. Eugene Skluzacek, in his doctoral dissertation (Ref 8), presented a very efficient numerical scheme for solving the integral form of the neutron transport equation. His efficient numerical solution relied on an "interpolation coefficient" developed by his advisor, George H. Nickel. This "interpolation coefficient" (Ref 8:53) was used in the integration over S to express the flux as a function of S rather than R (see Figure 2, page 21). The initial plan was to apply this same numerical scheme to the integration over S in Peierls' integral equation for the thermal radiation flux.

Two very important differences exist between Peierls' integral equation and the integral form of the neutron transport equation. These two differences greatly complicate using the same numerical scheme. The first difference is in the cross sections. The neutron cross section is uniform between radial mesh boundaries, while the photon opacity is non-uniform. Not only is the photon opacity non-uniform, but it also depends on one of the dependent variables, namely the kinetic air temperature. The second difference comes in the time dependence of the neutron transport problem compared to the x-ray transport problem. In the case of neutron transport, the time dependent problem can be transformed into a stationary problem by assuming an exponential growth rate and solving

the resulting eigenvalue problem. For the x-ray transport model developed in this study, the time dependence -- more specifically, the retarded time dependence -- must be numerically dealt with to obtain an accurate solution to the model.

The equation for the thermal radiation flux,

$$F_t(R,t) = \int dVOL \frac{\rho\kappa_t\left[\frac{T_B}{T(R',t-S/c)}\right]^3 caT(R',t-S/c)^4}{4\pi S^2}$$

$$\times\ e^{-\int_0^S \rho\kappa_t\left[\frac{T_B}{T(R',t-S'/c)}\right]^3 dS'} \tag{4.1}$$

is now re-examined to determine the effect of the retarded time dependence, and the opacity temperature dependence, on a numerical solution. To avoid a discontinuity which arises when $R' = R$, S is chosen as the variable of integration. The differential volume element becomes

$$dVOL = S^2 \sin\theta\, d\theta\, d\phi\, dS \tag{4.2}$$

where θ is the angle between R and S . Since the problem is symmetric in the azimuthal angle, the ϕ

integration can be evaluated to give

$$dVOL = 2\pi S^2 \sin\theta \, d\theta \, dS \tag{4.3}$$

The integration over θ can easily be handled if a transformation is made to an integration over $\mu = \cos\theta$, since

$$\int_0^{\pi} \sin\theta \, d\theta f(\theta) = \int_{-1}^{+1} d\mu f(\mu) \tag{4.4}$$

Integrals of this type are accurately approximated by Gaussian quadrature, giving

$$\int_{-1}^{+1} d\mu f(\mu) \simeq \sum_{\ell=1}^{L} \omega_\ell \, f(\mu_\ell) \tag{4.5}$$

where

ω_ℓ = quadrature weights

μ_ℓ = direction cosines.

The volume integral has now been reduced by azimuthal symmetry and Gaussian quadrature to a weighted sum of L one-dimensional integrals over S, giving

$$F_t(R,t) = \tfrac{1}{2}\rho\kappa_t c a T_B^{\,3} \sum_{\ell=1}^{L} \omega_\ell \int_0^{S_{max}} dS\,T(R',t-S/c)$$

$$\times \; e^{-\int_0^S \rho\kappa_t \left[\frac{T_B}{T(R',t-S'/c)}\right]^3 dS'} \qquad (4.6)$$

In the neutron transport model, the exponential growth can be incorporated into the exponential attenuation term by defining a new cross section (Ref 8:17). Since the neutron cross section is uniform between radial shells, it is possible to incorporate the "interpolation coefficient" for the flux, and then, by a change of variables, get an integral of the form

$$\int_a^b Z^n e^{-Z}\, dZ \qquad (4.7)$$

This integral is just the partial gamma function which has an analytic solution.

In Equation (4.6) for the thermal radiation flux, the opacity depends on the temperature. Since the temperature depends on position and time, the exponential integral cannot be solved analytically in its present form. If the kinetic air temperature was defined on the shell boundaries

and varied linearly with R between shell boundaries, then the integration over S would require interpolation in both position and time for the air temperature. The crossing of shell boundaries at retarded times during an integration over S is not likely to coincide to times when the kinetic air temperature has previously been determined. The "interpolation coefficients" require modifications to account for the dependence of the air temperature, and hence the opacity, on position and time. The original difference scheme which worked very efficiently for the transport of neutrons was found to be too difficult to apply efficiently to solving this x-ray transport equation. For this reason, a numerical solution to this model was not reached. The equations defining the streaming radiation flux and material temperature of air both lend themselves to more efficient numerical solutions and do not introduce any specific numerical complications.

V. Conclusions and Recommendations

A theoretical x-ray transport model has been developed to describe the radiative transport process which takes place following the release of a large amount of x-ray energy in the atmosphere. The model, based on a form of Peierls' integral equation, was intended to be a compromise between simple diffusion theory models and accurate transport theory models. The conclusions, drawn from the analysis in Section IV, will be presented first, followed by the recommendations.

CONCLUSIONS

Radiative transport, as described with a form of Peierls' integral equation, accurately models the physical processes which take place when a large amount of x-ray energy is released in the atmosphere. The integral approach to solving for the thermal radiation flux accurately takes into account the nonlocal and retarded time dependent characteristics of the radiation field. Since diffusion theory is limited in its ability to treat the streaming radiation flux, two distinct phases are required to model the radiative transfer based on diffusion theory. The model developed in this study provides a smooth transition from growth of the ionized sphere due to streaming radiation

to growth due to thermal radiation. Unlike diffusion theory models, the accuracy of a solution to this model is not affected by the nearness of a boundary or the size of the system in comparison to the photon mean free path. Instead of ignoring spatial gradients, this model calculates the spatial gradients, giving more detail and resolution to the resulting values of the streaming radiation flux, thermal radiation flux, and material temperature of air. From a theoretical standpoint, this model should be considerably more accurate than diffusion theory models.

A numerical solution to this x-ray transport model is greatly complicated due to time retardation and the temperature dependence of the opacity. A numerical difference scheme that had worked very efficiently for the integral form of the neutron transport equation was found to require too many approximations to account for the opacities temperature dependence and time retardation. These approximations served to increase the complexity of the numerical solution, while decreasing its efficiency. The final conclusion was that an efficient numerical solution to this model could not be obtained with the originally planned numerical difference scheme. There was not enough time to devise an alternative difference scheme that would solve the model efficiently, without making simplifying assumptions and reducing the model's accuracy. Given more time, it is possible that an

efficient numerical solution to the model might be worked out.

RECOMMENDATIONS

The following recommendations present the author's view concerning extensions of this research and possible applications for this x-ray transport model.

1. Appendix A presents an algorithm for solving a simplified version of the model, where the kinetic air temperature at any time t, is defined between shell boundaries and assumed uniform between shell boundaries. Continued work is needed to devise an algorithm and a set of difference equations for the more difficult problem where the kinetic air temperature is defined on the shell boundaries and assumed to vary linearly between shell boundaries. From the set of difference equations, a numerical solution can be obtained and a measure of the model's accuracy and efficiency determined by comparison to other x-ray transport benchmark calculations.

2. Throughout this model, it was assumed that the opacity of air had an inverse cubic temperature dependence. This assumption, taken from Pomraning's model (Ref 4:223), turned out to be a critical assumption, as it caused most of the numerical complications. It is recognized that the photoelectric cross section is inversely proportional to

the cube of the incoming photon energy, but the fact that the opacity has an inverse temperature dependence is not obvious. Although there is no reason to doubt Pomraning's assumption, the question has been raised as to justification of the assumption. Continued work on the numerical solution to this model should include justifying this assumption and/or investigating other alternative approaches to determining the opacity of air.

3. If an efficient numerical solution can be developed for this model, then consideration should be given to using the output from this model as the input to a hydrodynamic model which develops and propagates the shock wave.

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Appendix A

Numerical Algorithm for Solving the Model

This appendix presents an algorithm for a numerical solution to this x-ray transport model. The algorithm is not intended to be a step-by-step computer implementation of a set of difference equations, but merely serves as an outline to indicate the logic and direction of flow for a computer program to follow. The algorithm will be preceded by a general description of a typical radial mesh, to include the radial dependence of the various quantities being solved for.

TYPICAL RADIAL MESH

A typical radial mesh would consist of a series of concentric, spherical shells whose boundaries can be defined by the relationship (Figure A-1),

$$r_{i+1} = r_i + \Delta r \tag{A.1}$$

Both the streaming radiation flux and the thermal radiation flux would be defined on the shell boundaries. It is assumed that between specific radii the streaming and thermal radiation fluxes vary linearly with r . The algorithm is much more difficult, and has not been worked out for the

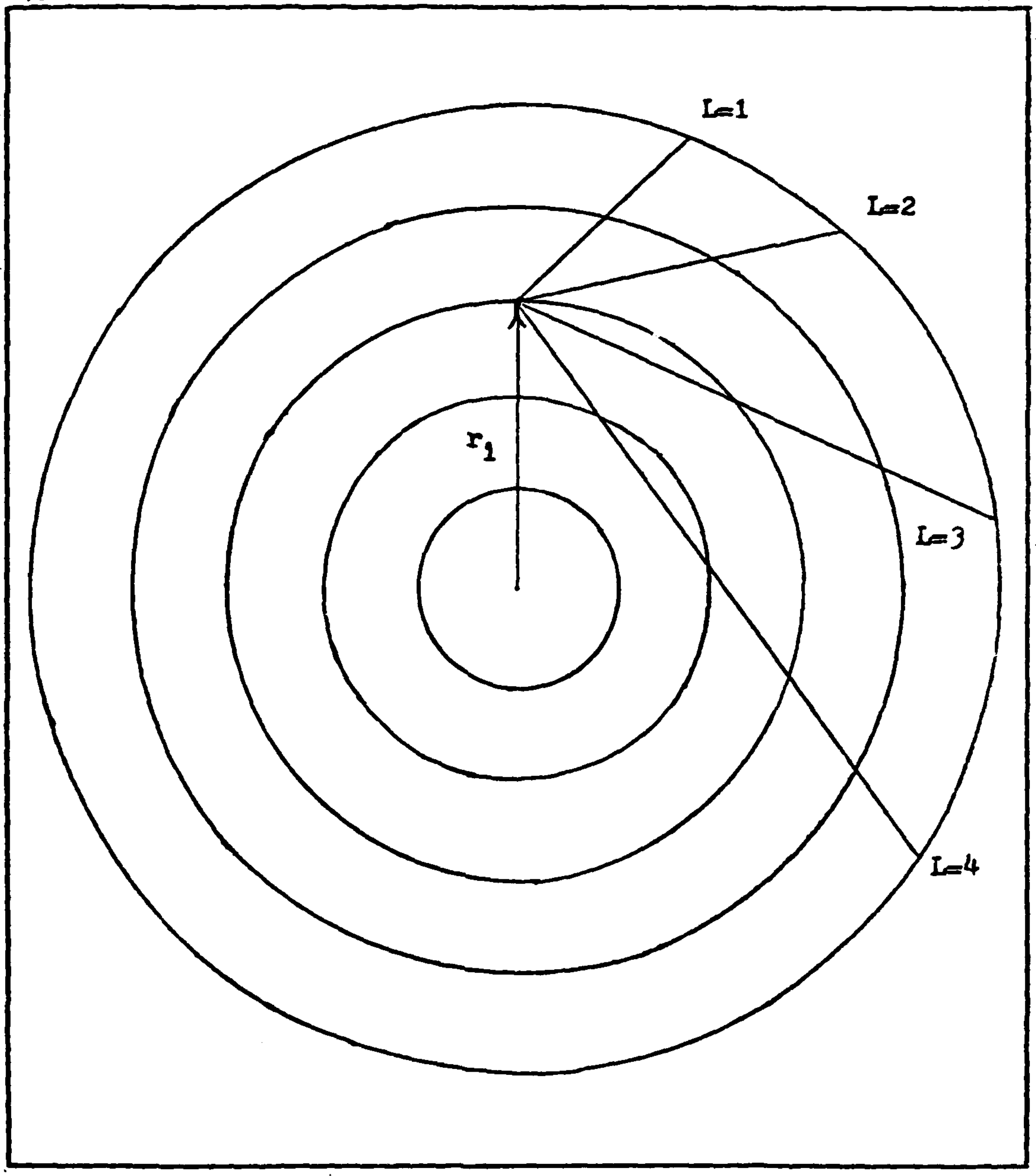

Figure A-1. Radial Mesh with Several Integration Rays

case when the kinetic air temperature is defined on the shell boundaries, and is assumed linear with r between shell boundaries. This algorithm will treat the simpler case of the kinetic air temperature being determined between shell boundaries, and assumed uniform between shell boundaries. Figure A-1 depicts a radial mesh along with several of the Gaussian quadrature rays that will be needed for the volume integration to determine the thermal radiation flux.

A typical x-ray transport problem might require 50 radial shells, each shell being 1.5 meters apart. To trace the radiative growth from time $t = 0$ to $t = 1.0 \times 10^{-6}$ sec would require at least 200 time steps. Usually, the time steps are no longer than the time it takes a photon to travel the width of a radial shell. The volume integral for the thermal radiation flux would require approximately ten $(L = 10)$ Gaussian quadrature rays to get acceptable convergence of the θ integration. For 50 radial shells and 200 time steps, a minimum of 30,000 memory locations would be required for the three dependent variables.

NUMERICAL ALGORITHM

The following algorithm lists in order the steps to be taken in solving this x-ray transport model. The algorithm is for the case when the time increments, Δt, are exactly equal to $\Delta r/c$.

STEP 1 Read in all the applicable constants and parameters. This includes Y , α , β , t_o , c , k , T_B , κ_s , κ_t , ρ , σ , a , and C_V .

STEP 2 Normalize the time dependence and determine a value for Z based on α , β , and t_o . An efficient two-point quadrature rule is presented by Pomraning for this normalization (Ref 6:23).

STEP 3 Read in the initial conditions. The air temperature, for all mesh regions and times can be initially set to standard atmospheric temperature. The thermal radiation flux, for all radii and times, can initially be set to zero. The streaming radiation flux can be set equal to zero for all radii (except $r = 0$) and times. Select a value for Δr , Δt , and calculate the mesh radii and times from

$$r_1 = 0 \qquad r_{i+1} = r_i + \Delta r$$

$$t_1 = 0 \qquad t_{n+1} = t_n + \Delta t \tag{A.2}$$

STEP 4 Increment the time index, n .

STEP 5 Set the radial index, i , equal to the time index, n .

STEP 6 Calculate $F_{s_i}^n$ from Eq (3.11).

STEP 7 Calculate T_i^n from Eq (3.18).

STEP 8 Calculate $F_{t_i}^n$ from Eq (3.15).

STEP 9 Repeat STEPS 6, 7, and 8, keeping the time index, n, constant while reducing the radial index, i, by one each time until F_s, T, and F_t have been calculated for all radii i, less than or equal to n. Then, go back to STEP 4 and increment the time index, and start the set of calculations over. The calculation continues until the final value of the time is reached.

ADDITIONAL COMMENTS

At late times, the calculation for the streaming radiation flux can be omitted when the source strength, $Yf(t)$, is negligibly small.

The time rate of change of the air temperature in Eq (3.18) can be replaced by a backward difference equation. The unknown air temperature will have to be solved with an iterative procedure. One approach is to use a Bolzano search which halves the interval of uncertainty each iteration.

While integrating on one of the Gaussian quadrature rays from $S = 0$ to S_{max}, in the calculation of the thermal radiation flux, the air temperature will change when either a new mesh region is entered or a retarded time is reached

for which a different air temperature applies. A test should be made which terminates the integration when either the contributions are negligibly small or a retarded time is reached that is negative.

Vita

Robert Paige Dickey was born on 29 November 1950 in Boston, Massachusetts. He is the son of Hume C. and Myrtle A. Dickey. He graduated from Whitman-Hansen Regional High School, Whitman, Massachusetts, in June 1968. In June 1972 he graduated from Lowell University, Lowell, Massachusetts with the degree of Bachelor of Science in Nuclear Engineering. Captain Dickey entered the Air Force in June 1972, having received his commission through the Reserve Officer Training Corps program. He then attended Undergraduate Navigator Training at Mather Air Force Base, California, receiving his navigator wings in April 1973. After navigator training, he completed transition training for the C-5A aircraft and was assigned to the 22nd Military Airlift Squadron, Travis Air Force Base, California. At Travis AFB he performed as a C-5A navigator, instructor navigator, flight examiner navigator, and command post senior controller until entering the School of Engineering, Air Force Institute of Technology, in August 1978.

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An x-ray transport model is developed which gives the streaming radiation flux, thermal radiation flux, and material energy of air, as a function of position and time, following the release of a large amount of x-ray energy in the atmosphere. The model is intended as a compromise between the simple diffusion theory models and the accurate transport theory models. It applies to the radiative growth which takes place at early times before hydrodynamic motion begins. The model assumes that air is heated by photoelectric absorptions to a

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BLOCK 20: ABSTRACT (Cont'd)

burnout temperature, the kinetic temperature at which the air molecules are completely ionized. The opacity of air is assumed very large at temperatures below the burnout temperature and very small at temperatures above the burnout temperature. Peierls' integral equation is used to calculate the flux of thermal radiation which builds up in the burned-out air. The integral equation considers both the nonlocal and retarded time-dependent characteristics of the radiation field. An efficient numerical solution to the model is greatly complicated due to the inverse cubic temperature dependence of the opacity and the retarded time dependence of the thermal radiation field. A numerical algorithm is presented for solving the model.